

ABSTRACT

Roihana Zulfa. 24020121140207. In Silico Study of the Potential of Black Rice (*Oryza sativa* L.) Anthocyanins as Antihypercholesterolemic Agents through Inhibition of Asialoglycoprotein Receptor 1 (ASGR1). Under the guidance of Sunarno dan Rizki Sandhi Titisari.

Hypercholesterolemia is a lipid metabolism disorder that increases the risk of cardiovascular disease; one of its causes is the excessive activity of Asialoglycoprotein Receptor 1 (ASGR1), which inhibits the expression of the Low-Density Lipoprotein Receptor (LDLR) in hepatocytes. Black rice (*Oryza sativa* L.) contains anthocyanin compounds with antioxidant and antiinflammatory properties, suggesting their potential as antihypercholesterolemic agents. This study aimed to analyze the potential of anthocyanin compounds from black rice (*Oryza sativa* L.) as antihypercholesterolemic agents through in silico inhibition of ASGR1. The methods employed included data collection from the PubChem and RCSB PDB databases, screening of bioactive compounds, and molecular docking using the PyRx program. All anthocyanin compounds satisfied Lipinski's Rule of Five, exhibited pharmacokinetic profiles suitable for oral drug candidates, and demonstrated low toxicity. The interactions of the anthocyanin compounds with the ASGR1 target protein formed hydrogen bonds at residues Gln239, Asp241, Glu252, and Asn264, as well as a hydrophobic interaction at residue Asp266, which play a crucial role in the activity and stability of the ASGR1 receptor. Cyanidin-3-O-glucoside exhibited the best inhibitory potential, with the most negative binding affinity value of -7.4 kcal/mol. These results demonstrate that black anthocyanin compounds (*Oryza sativa* L.) have the potential to act as antihypercholesterolemic agents through in silico inhibition of the ASGR1 protein, with cyanidin-3-O-glucoside identified as a potential candidate among the anthocyanin compounds tested.

Keywords: Hypercholesterolemia, black rice, anthocyanin, molecular docking